Spin Instabilities and Quantum Phase Transitions in Integral and Fractional Quantum Hall States

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The inter-Landau-level spin excitations of quantum Hall states at filling factors $\nu = 2$ and $\frac{4}{3}$ are investigated by exact numerical diagonalization for the situation in which the cyclotron ($\hbar\omega_c$) and Zeeman ($E_{\rm Z}$) splittings are comparable. The relevant quasiparticles and their interactions are studied, including stable spin wave and skyrmion bound states. For $\nu = 2$, a spin instability at a finite value of $\varepsilon = \hbar\omega_c - E_{\rm Z}$ leads to an abrupt paramagnetic to ferromagnetic transition, in agreement with the mean-field approximation. However, for $\nu = \frac{4}{3}$ a new and unexpected quantum phase transition is found which involves a gradual change from paramagnetic to ferromagnetic occupancy of the partially filled Landau level as ε is decreased.

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The elementary excitations of a two-dimensional electron gas (2DEG) with energy quantized into Landau levels (LL's) by a high magnetic field B have been extensively studied for decades. The charge excitations govern transport, including the integral and fractional quantum Hall effects (IQHE and FQHE) [1]. The spin excitations appear in the context of spin waves (SW's) [2], spin instabilities and related quantum phase transitions (QPT's) [3,4], and skyrmions [5,6].

In this letter we study spin excitations of IQH and FQH systems with densities ϱ corresponding to the filling factors $\nu = 2\pi\varrho\lambda^2 \approx 2$ and $\frac{4}{3}$ (here, $\lambda = \sqrt{\hbar c/eB}$ is the magnetic length). The cyclotron ($\hbar\omega_c$) and Zeeman ($E_{\rm Z}$) splittings are assumed comparable and much larger than the Coulomb energy $E_{\rm C} = e^2/\lambda$. In this situation, the spin excitations couple two partially filled LL's with different orbital indices, $n = 0$ and 1. These LL's, denoted by $|0\!\uparrow\rangle$ and $|1\!\downarrow\rangle$, are separated by a small gap $\varepsilon = \hbar\omega_c - E_{\rm Z} \ll E_{\rm C}$ from each other and by large gaps $\sim \hbar\omega_c \gg E_{\rm C}$ from the lower, filled $|0\!\downarrow\rangle$ LL and from the higher, empty LL's, as shown schematically in Fig. 1(c).

For the $\nu = 2$ ground state (GS), it is well-known [3] that a spin-flip instability occurs at a finite gap ε and wave vector k. In the mean-field approximation (MFA), this instability signals an abrupt, interaction-induced QPT from paramagnetic (P; $|0\!\downarrow\rangle$ and $|0\!\uparrow\rangle$ filled) to ferromagnetic (F; $|0\!\downarrow\rangle$ and $|1\!\downarrow\rangle$ filled) occupancy. Our numerical results confirm the validity of the MFA for $\nu = 2$. However, for $\nu = \frac{4}{3}$ they predict a new and unexpected P→F QPT that occurs through a series of intermediate GS's involving increasing number of spin flips as ε is decreased from $\varepsilon_{\rm P}$ to $\varepsilon_{\rm F}$ (the lower and upper boundaries of ε for the P and F occupancies, respectively).

The model is the same as that used earlier [6,7], except that now the spin excitations connect two different LL's. The electrons are confined to a spherical surface [8] of radius R. The radial magnetic field B is due to a monopole of strength $2Q$, defined in units of the flux quantum $\phi_0 = hc/e$ so that $4\pi R^2 B = 2Q\phi_0$ and $R^2 = Q\lambda^2$. The single-electron states are labeled by angular momentum $l = Q + n$ and its projection m.

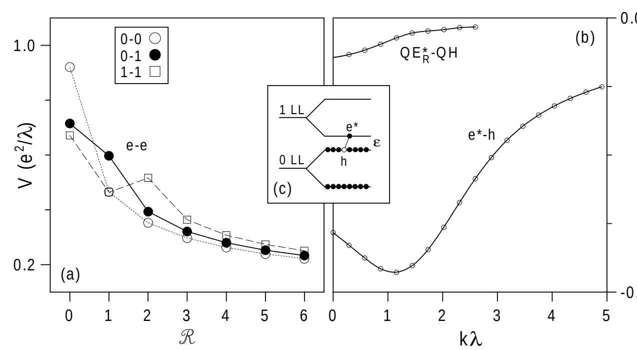

FIG. 1. The Coulomb pseudopotentials V for the pair of: (a) electrons in the $n = 0$ and 1 LL's, and (b) reversed-spin electron (e^*) or quasielectron (QE$^*_{\rm R}$) in the $n = 1$ LL and hole (h) or quasihole (QH) in the $n = 0$ LL. (c) Schematic of the LL structure at $\nu = 2$, with the h and e^* quasiparticles.

Only the partially filled $|0\!\uparrow\rangle$ and $|1\!\downarrow\rangle$ LL's (labeled by pseudospin $s =\uparrow$ and $\downarrow$) are included in the calculation, and the filled, rigid $|0\!\downarrow\rangle$ LL enters through the exchange energy Σ_{10}. The ratio $\varepsilon/E_{\rm C}$ is taken as an arbitrary parameter. Although we do not discuss the effect of the finite width w of a realistic 2DEG [6] and only present the results obtained using the pseudopotential $V(\mathcal{R})$ (interaction energy as a function of relative pair angular momentum [9]) for $w = 0$, shown in Fig. 1(a), we have checked that our conclusions remain valid for $w \le 5\lambda$.

The Hamiltonian H for electrons confined to the $|0\!\uparrow\rangle$ and $|1\!\downarrow\rangle$ LL's contains the single-particle term ($\varepsilon - \Sigma_{10}$) and the intra- and inter-LL two-body interaction matrix elements $\langle m_1 s, m_2 s'|V|m_3 s', m_4 s\rangle$ calculated for the Coulomb potential $V(r) = e^2/r$ and connected with pseudopotentials $V_{ss'}(\mathcal{R})$ shown in Fig. 1(a) through the Clebsch–Gordan coefficients (on a sphere, $\mathcal{R} = 2l - L$ where $L = \mathbf{l}_1 + \mathbf{l}_2$ is pair angular momentum).

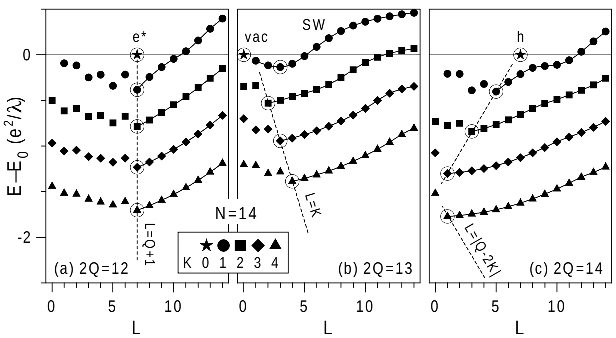

FIG. 2. The excitation energy spectra (energy E as a function of angular momentum L) of $N = 14$ electrons in the $|0\uparrow\rangle$ and $|1\downarrow\rangle$ LL's calculated on a sphere for the monopole strengths $2Q = 12$ (a), 13 (b), and 14 (c), corresponding to the filling factors $\nu \approx 2$. The lowest $|0\downarrow\rangle$ LL is filled. E_0 is the energy of the lowest paramagnetic ($K = 0$) state, and dashed lines mark the lowest states for different values of K.

Hamiltonian H is diagonalized in the basis of N-electron Slater determinants $|m_1 s_1 \dots m_N s_N\rangle$. This allows automatic resolution of the projection of pseudospin ($S_z = \sum s_i$) and of angular momentum ($L_z = \sum m_i$). The quantum number $K = \frac{1}{2}N + S_z$ measures the number of reversed spins relative to the paramagnetic configuration. The length of angular momentum (L) is resolved numerically in the diagonalization of each (S_z, L_z) Hilbert subspace. The length of pseudospin is not a good quantum number because of the pseudospin-asymmeteric interactions. The results obtained on Haldane sphere are easily converted to the planar geometry, where L and L_z are appropriately [10] replaced by the total and center-of-mass angular momentum projections, M and $M_{\rm CM}$.

Let us begin with the discussion of the IQH regime. Fig. 2 presents the spin-excitation spectra for $N = 14$, at the filling factors equal to or different by one flux from $\nu = 2$. Only the lowest state is shown for each K and L. The energy E is measured from the lowest paramagnetic state (at $E = E_0$) and excludes the inter-LL gap ε. Symbols e^* and h denote reversed-spin electrons (particles in the $|1\downarrow\rangle$ LL) and holes (vacancies in the $|0\uparrow\rangle$ LL) created in the "vacuum" state (completely filled $|0\uparrow\rangle$ LL).

The excitation spectrum of the "vacuum" state is shown in Fig. 2(b). The $K = 1$ band is a SW; in a finite system it has $L = 1$ to N, as follows from addition of the e^* and h angular momenta, $l_{e^*} = Q + 1$ and $l_h = Q$. In an infinite system, the continuous SW dispersion is given by [2] $E_{\rm SW}(k) = E_0 + \frac{1}{2}E_{\rm C}\sqrt{\pi/2}\,\{1 - \exp(-\kappa^2)[(1 + 2\kappa^2)I_0(\kappa^2) - 2\kappa^2 I_1(\kappa^2)]\}$, where $\kappa = \frac{1}{2}k\lambda$, I_0 and I_1 are the modified Bessel functions, and $k = L/R$. $E_{\rm SW}(k)$ starts at $E = E_0$ for $k = 0$ and has a minimum at $k \approx 1.19\lambda^{-1}$ and $E \approx E_0 - 0.147\,E_{\rm C}$. The vanishing of SW energy at $k = 0$ is the result of exact cancellation of the sum of e^* and h exchange self-energies, $-\Sigma_{10} + \Sigma_{00}$, by the e^*–h attraction V_{e^*h} at $k = 0$; the entire e^*–h pseudopotential is shown in Fig. 1(b).

The energy spectra corresponding to consecutive spin flips ($K = 2, 3, \dots$) at $\nu = 2$ all contain low-energy bands at $L \ge K$. For each K, the GS's (open circles) have $L = K$ and their energies fall on a nearly straight line, $E(K)$. These GS's are therefore denoted by $\mathcal{W}_K = K \times {\rm SW}$ and interpreted as containing K SW's with parallel angular momenta each of length $L = 1$, similar to the $L = K$ SW condensates at $\nu = 1$ [6]. The new feature at $\nu = 2$ is the SW–SW attraction (due to a finite dipole moment of an inter-LL SW) giving rise to a negative slope of $E(K)$.

Let us now turn to Fig. 2(a) and (b) showing spin excitation spectra in the presence of an e^* or h. The series of GS's for $K \ge 1$ (open circles) are charged bound states, similar to the skyrmions and anti-skyrmions at $\nu = 1$. Their angular momenta result from simple vector addition of l_{e^*} and l_h. For $\mathcal{S}_K^- = K \times {\rm SW} + e^*$ and $\mathcal{S}_K^+ = K \times {\rm SW} + h$ we get $L = (\mathbf{l}_{e^*})^{K+1} \oplus (\mathbf{l}_h)^K = Q + 1$ and $L = (\mathbf{l}_{e^*})^K \oplus (\mathbf{l}_h)^{K+1} = |Q - 2K|$, respectively. In both cases, finite $L \propto Q$ means massive LL degeneracy, as expected for charged particles in a magnetic field.

Let us check if the negative SW energy at $k \approx 1.19\lambda^{-1}$ or the SW–SW attraction causes instability of the $\nu = 2$ GS towards the formation of one or more SW's when ε is decreased. The single-SW instability has been ruled out by Giuliani and Quinn [3] who showed that it is preempted by a direct transition to the ferromagnetic GS. The critical value of ε for this P→F QPT is expressed through the involved self-energies, $\varepsilon_0 = \Sigma_{10} + \frac{1}{2}(\Sigma_{11} - \Sigma_{00}) = \frac{3}{8}\sqrt{\pi/2}\,E_{\rm C} \approx 0.47\,E_{\rm C}$, and it is larger than $E_0 - E_{\rm SW}$. Since the energy per spin flip, $[E(K) - E_0]/K$, is smaller for the SW condensates and skyrmions than for a single SW, we still need to check for a possible vac→$\mathcal{W}_K$, e^*→$\mathcal{S}_K^-$, or h→$\mathcal{S}_K^+$ instability. Fig. 3(a) shows that despite evident SW–SW, SW–e^*, and SW–h attraction ($\delta E = E - E_0 + K\varepsilon_0$ is the energy to create K SW's in "vacuum" or in the presence of an e^* or h), the $\mathcal{W}_K$ and $\mathcal{S}_K^\pm$ energies are all positive at $\varepsilon = \varepsilon_0$. This precludes spin instability at $\nu = 2$ other than the direct P→F transition (skipping the states with intermediate spin).

To translate our finite-size spectra to the case of an infinite 2DEG, in Fig. 3(b) we have plotted the energies of the SW condensate calculated for different electron numbers, $N \le 14$. Clearly, all data fall on the same curve when $\delta E/\sqrt{N}$ is plotted as a function of "relative" spin polarization, $\zeta = K/N$. This resembles the insensitivity to N of the $\delta E(\zeta)$ curves for the SW condensates at $\nu = 1$, except that now $\delta E \propto N^{1/2}$ (rather than $\propto N^0$).

The data of Fig. 3 allows calculation of the SW binding energies, $U_K = [E(K-1) - E_0] + [E_{\rm SW} - E_0] - [E(K) - E_0]$, for the $\mathcal{W}_K$ and $\mathcal{S}_K^\pm$ states. Because of the SW–SW attraction, all these energies increase in a similar way as a function of K, in contrast to $\nu = 1$ where U_K decreased for skyrmions and vanished for the SW condensate.

Let us now turn to the FQH regime. At $\nu = \frac{4}{3}$, which occurs for $2Q = 3(N-1)$, and for sufficiently large ε,

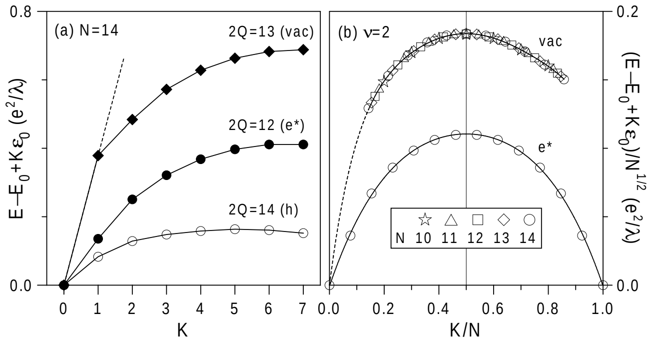

FIG. 3. (a) The energy of skyrmions, anti-skyrmions, and spin-wave condensates of Fig. 2, plotted as a function of K. The gap ε is set to the value ε_0 at which the paramagnetic ($K = 0$) and ferromagnetic ($K = N$) configurations are degenerate. (b) The energy of spin-wave condensates calculated for $N = 10$ to 14, rescaled by $\sqrt{N}$, and plotted as a function of $\zeta = K/N$. The skyrmion curve is shown for comparison.

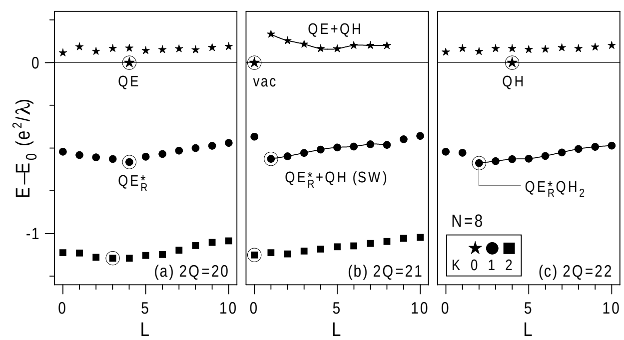

FIG. 4. Same as Fig. 2, but for $N = 8$ electrons and for the monopole strengths $2Q = 20$ (a), 21 (b), and 22 (c), corresponding to the filling factors $\nu \approx \frac{4}{3}$.

the N electrons in the $|0{\uparrow}\rangle$ LL form the Laughlin $\nu = \frac{1}{3}$ state. These electrons, each with angular momentum $l = Q$, can be converted into an equal number of composite fermions (CF's) [11] each with effective angular momentum $l^* = l - (N-1)$, exactly filling their effective LL. The elementary charge excitations of the $\nu = \frac{1}{3}$ state are two types of Laughlin quasiparticles (QP's), quasielectrons (QE's) and quasiholes (QH's), corresponding to an excess particle in an (empty) excited CF LL, or a hole in the (filled) lowest CF LL, respectively.

The reversed-spin quasielectrons ($\mathrm{QE_R}$'s) [7,12] do not occur at $\nu = \frac{4}{3}$ because of the electrons completely filling the $|0{\downarrow}\rangle$ LL. This causes a difference between the SW's at $\nu = \frac{4}{3}$ and $\frac{1}{3}$, similar to that between $\nu = 2$ and 1. At $\nu = \frac{1}{3}$ the SW consisted of a QH and a $\mathrm{QE_R}$, and at $\nu = \frac{4}{3}$ it is formed by a QH and a different reversed-spin QP that we will denote by $\mathrm{QE_R^*}$.

The $\mathrm{QE_R^*}$ has the same electric charge of $-\frac{1}{3}e$ as QE or $\mathrm{QE_R}$ but it belongs to an excited electron LL, $|1{\downarrow}\rangle$. Similar to the case for QH, QE, and $\mathrm{QE_R}$, the existence and stability of the $\mathrm{QE_R^*}$ depend on the validity of the CF transformation for the underlying system of $N-1$ electrons in the $|0{\uparrow}\rangle$ LL and one electron in the $|1{\downarrow}\rangle$ LL. This requires Laughlin correlations between the $|1{\downarrow}\rangle$ electron and the $|0{\uparrow}\rangle$ electrons, i.e. the occurrence of a Jastrow prefactor, $\prod_{ij}(z_i^{(0)} - z_j^{(1)})^\mu$, in the many body wave function, with $\mu = 2$ for $\nu = (1+\mu)^{-1} = \frac{1}{3}$. Such correlations result from short-range e–e repulsion, and the criterion is [13,14] that the pseudopotential V must decrease more quickly than linearly as a function of the average square e–e separation $\langle r^2\rangle$. On a plane (or on a sphere for $\langle r^2\rangle \ll R^2$, i.e. for $\mathcal{R} \ll Q$) this is equivalent to a superlinear decrease of V as a function of $\mathcal{R}$.

It is clear from Fig. 1(a) that the Coulomb inter-LL pseudopotential $V_{01}(\mathcal{R})$ is a short-range repulsion for $\mathcal{R} \geq \mathcal{R}_0 = 1$. This implies the Jastrow prefactors with $\mu > \mathcal{R}_0 = 2, 3, \ldots$ in the $|0{\uparrow}\rangle^{N-1} \oplus |1{\downarrow}\rangle$ wave function, if only $\nu \leq (1+\mu)^{-1}$. In particular, this establishes the $\mathrm{QE_R^*}$ as a stable reversed-spin QP of the $\nu = \frac{4}{3}$ state, in analogy to the reversed-spin electron, e^*, at $\nu = 2$. The angular momentum of $\mathrm{QE_R^*}$ on a sphere can be obtained in the two-component CF picture [15] appropriate for $\nu = \frac{1}{3}$, i.e. with both 0–0 and 0–1 Laughlin correlations modeled by attachment of two flux quanta to each electron. The resulting CF angular momenta are $l_{\rm QH} = Q^*$ and $l_{\rm QE} = l_{\rm QE_R^*} = Q^* + 1$, where $Q^* = Q - (N-1)$.

The excitation spectra at filling factors equal to or different by one flux from $\nu = \frac{4}{3}$ are displayed in Fig. 4. $N = 8$ in each frame, and the values of $2Q$ are 20, 21, and 22, corresponding to the following GS's at $K = 0$: (a) QE at $L = 4$, (b) "vacuum" (filled CF LL) with $L = 0$, and (c) QH at $L = 4$. The low-energy charge excitations for $2Q = 21$ form the magnetoroton (QE+QH) band. The low-energy spin excitations with $K = 1$ are the following: (a) $\mathrm{QE_R^*}$ at $L = l_{\rm QE_R^*} = 4$ for $2Q = 20$, (b) the SW ($\mathrm{QE_R^*}$+QH) band with L going from 1 to $N = 8$, as follows from vector addition of $l_{\rm QH}$ and $l_{\rm QE_R^*}$, for $2Q = 21$, and (c) a band of $\mathrm{QE_R^*}$+$\mathrm{QH_2}$ states with a bound GS denoted as $\mathrm{QE_R^*QH_2}$ for $2Q = 22$.

To draw analogy with Fig. 2, QE corresponds to an electron in the $|1{\uparrow}\rangle$ LL (not shown because of high energy), $\mathrm{QE_R^*}$ to e^*, QH to h, and $\mathrm{QE_R^*QH_2}$ to $\mathcal{S}_1^+$. The latter state is the only "skyrmion" at $\nu = \frac{4}{3}$. The $\mathcal{S}_K^-$ states with $K \geq 1$ and $L = Q^* + 1$ or the $\mathcal{S}_K^+$ states with $K \geq 2$ and $L = |Q^* - 2K|$ do not occur because of the weakened Coulomb repulsion at short range in the excited LL. As shown in Fig. 1(a), the linear behavior of $V_{11}(\mathcal{R})$ between $\mathcal{R} = 1$ and 5 prevents Laughlin correlations for two or more electrons in the $n = 1$ LL. This invalidates the CF model and causes break-up of $\mathrm{QE_R^*}$'s when two of them approach each other (at this point, pairing of electrons in the $n = 1$ LL occurs [14,16]). For the same reason, no $\mathcal{W}_K$ states at $L = K$ appear in Fig. 4(b) for $K > 1$.

Even more significant in Fig. 4 than the absence of $\mathcal{S}_K^\pm$ and $\mathcal{W}_K$ states is the large and negative SW energy $E_{\rm SW}^*(k)$ at $\nu = \frac{4}{3}$. This is in striking contrast

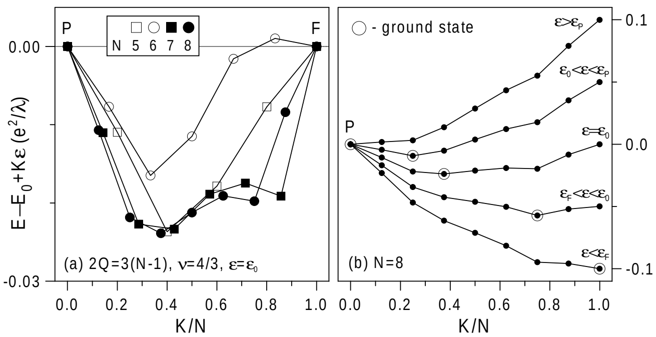

FIG. 5. (a) Same as Fig. 3(b), but for the filling factor $\nu = \frac{4}{3}$. (b) Data for $N = 8$ plotted for different values of ε.

to the $\nu = 2$ case, and it is explained as follows. The SW energy is the sum of the QE_R^* and QH self-energies and the QE_R^*–QH attraction. Of these three terms, only the QE_R^* self-energy, $-\Sigma_{10} = -\frac{1}{2}\sqrt{\pi/2}\,E_\mathrm{C}$, is the same at $\nu = 2$ and $\frac{4}{3}$, while the QH self-energy Σ_{00}^* and the QE_R^*–QH pseudopotential $V_{\mathrm{QE}_\mathrm{R}^*\mathrm{QH}}(k)$ are both reduced (because of only partial filling of the $|0\!\uparrow\rangle$ LL and the fractional QP charge, respectively). As a result, the large and negative $-\Sigma_{10}$ term becomes dominant in $E_\mathrm{SW}^*(k)$. Note that even without knowing analytic expressions for Σ_{00}^* or $V_{\mathrm{QE}_\mathrm{R}^*\mathrm{QH}}(k)$, the fact that $V_{\mathrm{QE}_\mathrm{R}^*\mathrm{QH}}(\infty) = 0$ allows the estimate of $V_{\mathrm{QE}_\mathrm{R}^*\mathrm{QH}}(k)$, as shown in Fig. 1(b), and of $\Sigma_{00}^* \approx 0.17\,E_\mathrm{C}$. Note that $V_{\mathrm{QE}_\mathrm{R}^*\mathrm{QH}}(0) \approx -0.11\,E_\mathrm{C} \approx \frac{1}{6}V_{e^*h}(0)$ and $\Sigma_{00}^* \approx \frac{1}{7}\Sigma_{00}$.

The dependence of the GS energy on $\zeta = K/N$ for $\nu = \frac{4}{3}$ is shown in Fig. 5(a). As in Fig. 3, ε is set to the value ε_0 for which the P and F configurations (at $\zeta = 0$ and 1) are degenerate. Clearly, (almost) all energies at $0 < \zeta < 1$ are negative. This effect does not depend on N; on the contrary, all data points for moderate values of ζ seem to to fall on the same curve, characteristic of an infinite (planar) system. Negative excitation energies imply that the paramagnetic Laughlin $\nu = \frac{4}{3}$ state is unstable toward flipping of only a fraction $\zeta < 1$ of spins when ε is decreased. This is illustrated in Fig. 5(b) where we display the data for $N = 8$ corresponding to five different values of ε. The gradual decrease of ε from ε_P to ε_F drives the system through entire series of GS's (open circles) with fractional values of ζ. This novel sequence of GS's are distinctly different from the abrupt P→F QPT found at $\nu = 2$, and they are not expected in the MFA.

In conclusion, our numerical study of small systems at $\nu = 2$ serves as a test of the MFA which predicts an abrupt interaction-induced P→F QPT associated with the spin-flip instability. This test should also be applicable to a similar instability and QPT which occurs for a bilayer [17] (where $\hbar\omega_c$ is replaced by the symmetric-antisymmetric splitting Δ_SAS). For the fractional $\nu = \frac{4}{3}$ state the series of spin-flip GS's between the para- and ferromagnetic states is a novel prediction that is susceptible to experimental observation.

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